Vanadium(V) complexes based on a bis(pyridine)-imine ligand (HL); synthesis and crystal structure of a dioxovanadium(V) complex involving a ligand cyclisation

Ligtenbarg, Alette G.J.; Spek, Anthony L.; Hage, Ronald; Feringa, Bernard

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#=============================================================================
data_global
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# 0. AUDIT DETAILS

_audit_creation_date                 'Wed Sep 23 15:53:22 1998'
_audit_creation_method               'PLATON <TABLE ACC> option'

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;   Dr. A.L. Spek
;
_publ_contact_author_address        # Address of author for correspondence
;
    Bijvoet Center for Biomolecular Research
    Department of Crystal and Structural Chemistry
    Utrecht University
    Padualaan 8
    3584 CH Utrecht
    The Netherlands
;
_publ_contact_author_email           'spea@chem.uu.nl'
_publ_contact_author_fax             '+31 30 2533940'
_publ_contact_author_phone           '+31 30 2532538'


#=============================================================================

data_s1720a

#=============================================================================

# 5. CHEMICAL DATA

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_chemical_compound_source           'see text'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 V   V    0.3005    0.5294
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 O   O    0.0106    0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 N   N    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=============================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting                Monoclinic
_symmetry_space_group_name_Hall      '-P 2ybc'
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_symmetry_space_group_name_H-M       'P 21/c'

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -x,1/2+y,1/2-z
 -x,-y,-z
 x,1/2-y,1/2+z

_cell_length_a                         7.0787(16)
_cell_length_b                          16.833(5)
_cell_length_c                          13.573(5)
_cell_angle_alpha                              90
_cell_angle_beta                        115.21(2)
_cell_angle_gamma                              90
_cell_volume                            1463.3(8)
_cell_formula_units_Z                   4
_cell_measurement_temperature          150

_exptl_crystal_description          block
_exptl_crystal_colour               yellow
_exptl_crystal_size_max            0.43
_exptl_crystal_size_mid            0.12
_exptl_crystal_size_min            0.10
_exptl_crystal_density_diffrn           1.676
_exptl_crystal_density_method       'Not Measured'
_exptl_crystal_F_000                     752
_exptl_absorpt_coefficient_mu           0.70
_exptl_absorpt_correction_type      delref
_exptl_absorpt_process_details      PLATON/DELABS
_exptl_absorpt_correction_T_min    0.143
_exptl_absorpt_correction_T_max    0.615

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# 7. EXPERIMENTAL DATA

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;
_diffrn_ambient_temperature         150
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type               'Mo K\a'
_diffrn_radiation_source            'Rotating Anode'
_diffrn_radiation_monochromator     graphite

_diffrn_measurement_device_type     'CAD4T'
_diffrn_measurement_method          'omega-scan'


# number of measured reflections (redundant set)
_diffrn_reflns_number                  6346
_diffrn_reflns_av_R_equivalents       0.1061
_diffrn_reflns_av_sigmaI/netI         0.1155
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_diffrn_reflns_limit_k_max              20
_diffrn_reflns_limit_l_min             -15
_diffrn_reflns_limit_l_max              16
_diffrn_reflns_theta_min              2.05
_diffrn_reflns_theta_max             26.50

# number of unique reflections
_reflns_number_total                   3006
# number of observed reflections (> n sig(I))
_reflns_number_gt                      1984
_reflns_threshold_expression         'I>2sigma(i)'

_computing_data_collection           'Locally modified CAD4-Version 5 Software'
_computing_cell_refinement           'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction            'HELENA (Spek, 1997)'
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_computing_structure_solution        'SHELXS86'
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_computing_publication_material      'PLATON (Spek, 1990)'

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# 8. REFINEMENT DATA

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'w=1/[\s^2^(Fo^2^)+(0.0561P)^2^] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment        'H-atom refinement: see text '
_refine_ls_extinction_method         none
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_refine_ls_abs_structure_Flack       none
_refine_ls_number_reflns                  3006
_refine_ls_number_parameters               226
_refine_ls_number_restraints                 0
_refine_ls_R_factor_all                 0.0992
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_refine_ls_wR_factor_ref                0.1415
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_refine_ls_goodness_of_fit_ref           1.017
_refine_ls_restrained_S_all              1.017
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_refine_diff_density_max                 0.592
_refine_diff_density_min                -0.547
_refine_diff_density_rms                 0.089

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# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
 V1     V  Uani   0.48998(12)   0.57903(4)   0.30698(5)     1.000   0.0219(2)
 O1     O  Uani     0.3133(5)  0.52189(16)    0.1818(2)     1.000   0.0253(8)
 O2     O  Uani     0.6349(5)  0.63471(18)    0.2711(2)     1.000   0.0279(9)
 O3     O  Uani     0.3167(5)  0.63423(16)    0.3241(2)     1.000   0.0262(9)
 N1     N  Uani     0.6258(5)  0.46685(18)    0.3526(2)     1.000   0.0198(9)
 N2     N  Uani     0.7201(5)  0.34208(18)    0.3607(2)     1.000   0.0184(9)
 N3     N  Uani     0.6724(6)  0.58101(19)    0.4825(2)     1.000  0.0238(10)
 C1     C  Uani     0.3605(7)    0.4666(2)    0.1253(3)     1.000  0.0217(11)
 C2     C  Uani     0.2540(7)    0.4697(3)    0.0107(3)     1.000  0.0272(12)
 C3     C  Uani     0.2977(7)    0.4159(3)   -0.0526(3)     1.000  0.0290(11)
 C4     C  Uani     0.4446(7)    0.3575(2)   -0.0060(3)     1.000  0.0274(14)
 C5     C  Uani     0.5466(7)    0.3516(2)    0.1063(3)     1.000  0.0254(12)
 C6     C  Uani     0.5034(7)    0.4043(2)    0.1738(3)     1.000  0.0206(11)
 C7     C  Uani     0.6107(6)    0.4031(2)    0.2921(3)     1.000  0.0207(11)
 C8     C  Uani     0.7459(6)    0.4491(2)    0.4597(3)     1.000  0.0194(11)
 C9     C  Uani     0.8104(6)    0.3712(2)    0.4686(3)     1.000  0.0191(11)
 C10    C  Uani     0.9354(7)    0.3194(2)    0.5528(3)     1.000  0.0228(11)
 C11    C  Uani     0.9658(7)    0.2433(2)    0.5288(3)     1.000  0.0287(14)
 C12    C  Uani     0.8611(7)    0.2148(2)    0.4192(3)     1.000  0.0276(14)
 C13    C  Uani     0.7407(7)    0.2624(2)    0.3392(3)     1.000  0.0249(14)
 C14    C  Uani     0.7792(6)    0.5152(2)    0.5338(3)     1.000  0.0195(11)
 C15    C  Uani     0.9054(7)    0.5146(2)    0.6466(3)     1.000  0.0237(11)
 C16    C  Uani     0.9135(7)    0.5836(3)    0.7038(3)     1.000  0.0282(14)
 C17    C  Uani     0.8032(7)    0.6500(3)    0.6519(3)     1.000  0.0298(14)
 C18    C  Uani     0.6830(7)    0.6464(2)    0.5402(3)     1.000  0.0275(14)
 H2     H  Uiso       0.15110      0.50940     -0.02290     1.000      0.0330
 H3     H  Uiso       0.22550      0.41910     -0.12960     1.000      0.0350
```

```
 H4     H  Uiso       0.47600      0.32130     -0.05070     1.000      0.0320
 H5     H  Uiso       0.64780      0.31100      0.13820     1.000      0.0300
 H10    H  Uiso       0.99820      0.33760      0.62610     1.000      0.0270
 H11    H  Uiso       1.05630      0.20910      0.58470     1.000      0.0340
 H12    H  Uiso       0.87820      0.16090      0.40360     1.000      0.0330
 H13    H  Uiso       0.66860      0.24230      0.26740     1.000      0.0300
 H15    H  Uiso       0.98220      0.46870      0.68220     1.000      0.0280
 H16    H  Uiso       0.99670      0.58500      0.78020     1.000      0.0340
 H17    H  Uiso       0.80910      0.69720      0.69140     1.000      0.0360
 H18    H  Uiso       0.60570      0.69200      0.50360     1.000      0.0330

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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
  V1       0.0234(4)  0.0206(3)  0.0224(3)   0.0031(3)   0.0105(3)   0.0018(3)
  O1      0.0252(16) 0.0258(14) 0.0239(14)  0.0003(11)  0.0095(13)  0.0042(14)
  O2      0.0260(17) 0.0359(16) 0.0228(14)  0.0020(12)  0.0113(13) -0.0010(15)
  O3      0.0290(18) 0.0240(14) 0.0288(14)  0.0026(12)  0.0153(14)  0.0049(14)
  N1      0.0208(19) 0.0181(15) 0.0184(15)  0.0013(13)  0.0063(14)  0.0018(15)
  N2      0.0175(18) 0.0179(15) 0.0205(16)  0.0001(13)  0.0088(15)  0.0010(14)
  N3        0.026(2) 0.0232(16) 0.0237(16) -0.0029(14)  0.0119(15) -0.0024(17)
  C1        0.027(2) 0.0208(19) 0.0221(19) -0.0015(15)  0.0151(18) -0.0028(18)
  C2        0.024(2)   0.030(2)   0.026(2)  0.0090(17)  0.0092(19)    0.002(2)
  C3        0.030(2)   0.034(2) 0.0209(19) -0.0003(18)  0.0089(19)   -0.006(2)
  C4        0.031(3)   0.029(2) 0.0203(19) -0.0043(17)  0.0092(19)   -0.005(2)
  C5        0.026(2)   0.023(2)   0.026(2)  0.0007(16)  0.0099(19)  0.0008(19)
  C6        0.022(2) 0.0214(19) 0.0181(18) -0.0007(14)  0.0082(17) -0.0029(18)
  C7        0.020(2)   0.023(2) 0.0201(18) -0.0005(15)  0.0095(18)  0.0002(17)
  C8        0.017(2) 0.0224(18) 0.0179(18)  0.0020(15)  0.0066(16) -0.0016(17)
  C9        0.014(2) 0.0242(19) 0.0163(18)  0.0004(15)  0.0037(16) -0.0025(17)
  C10       0.019(2)   0.030(2) 0.0190(19)  0.0034(16)  0.0078(17) -0.0007(19)
  C11       0.026(3)   0.027(2)   0.031(2)  0.0085(18)    0.010(2)    0.003(2)
  C12       0.030(3) 0.0213(19)   0.034(2)  0.0004(17)    0.016(2)    0.000(2)
  C13       0.029(3) 0.0184(19)   0.027(2) -0.0059(16)  0.0116(19) -0.0033(19)
  C14       0.015(2) 0.0217(19) 0.0237(19)  0.0003(15)  0.0102(17) -0.0001(17)
  C15       0.025(2)   0.029(2) 0.0182(19)  0.0030(16)  0.0102(18) -0.0045(19)
  C16       0.029(3)   0.036(2)   0.024(2) -0.0040(19)  0.0154(19)   -0.011(2)
  C17       0.037(3)   0.025(2)   0.037(2) -0.0092(18)    0.025(2)   -0.008(2)
  C18       0.029(3)   0.024(2)   0.030(2)  0.0007(17)    0.013(2)    0.002(2)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
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_geom_bond_distance
_geom_bond_site_symmetry_1
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_geom_bond_publ_flag
 V1      O1         1.888(3)                    .       .                  yes
 V1      O2         1.610(4)                    .       .                  yes
 V1      O3         1.632(4)                    .       .                  yes
 V1      N1         2.090(3)                    .       .                  yes
 V1      N3         2.173(3)                    .       .                  yes
 O1      C1         1.336(5)                    .       .                  yes
 N1      C7         1.328(5)                    .       .                  yes
```

```
 N1      C8        1.368(5)                    .       .               yes
 N2      C7        1.381(5)                    .       .               yes
 N2      C9        1.413(4)                    .       .               yes
 N2      C13       1.393(5)                    .       .               yes
 N3      C14       1.355(5)                    .       .               yes
 N3      C18       1.334(5)                    .       .               yes
 C1      C2        1.411(5)                    .       .               no
 C1      C6        1.410(6)                    .       .               no
 C2      C3        1.371(7)                    .       .               no
 C3      C4        1.374(6)                    .       .               no
 C4      C5        1.385(5)                    .       .               no
 C5      C6        1.399(6)                    .       .               no
 C6      C7        1.455(5)                    .       .               no
 C8      C9        1.377(5)                    .       .               no
 C8      C14       1.450(5)                    .       .               no
 C9      C10       1.410(5)                    .       .               no
 C10     C11       1.361(5)                    .       .               no
 C11     C12       1.433(5)                    .       .               no
 C12     C13       1.326(5)                    .       .               no
 C14     C15       1.406(5)                    .       .               no
 C15     C16       1.385(6)                    .       .               no
 C16     C17       1.374(7)                    .       .               no
 C17     C18       1.388(5)                    .       .               no
 C2      H2          0.9498                    .       .               no
 C3      H3          0.9494                    .       .               no
 C4      H4          0.9506                    .       .               no
 C5      H5          0.9505                    .       .               no
 C10     H10         0.9511                    .       .               no
 C11     H11         0.9505                    .       .               no
 C12     H12         0.9511                    .       .               no
 C13     H13         0.9492                    .       .               no
 C15     H15         0.9499                    .       .               no
 C16     H16         0.9500                    .       .               no
 C17     H17         0.9494                    .       .               no
 C18     H18         0.9507                    .       .               no

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 O1      V1      O2      106.70(14)            .       .       .       yes
 O1      V1      O3       99.68(15)            .       .       .       yes
 O1      V1      N1       81.44(12)            .       .       .       yes
 O1      V1      N3      148.28(13)            .       .       .       yes
 O2      V1      O3      109.02(16)            .       .       .       yes
 O2      V1      N1      110.10(16)            .       .       .       yes
 O2      V1      N3       99.50(15)            .       .       .       yes
 O3      V1      N1      138.68(15)            .       .       .       yes
 O3      V1      N3       88.10(14)            .       .       .       yes
 N1      V1      N3       72.87(12)            .       .       .       yes
 V1      O1      C1        129.8(3)            .       .       .       yes
 V1      N1      C7        129.9(2)            .       .       .       yes
 V1      N1      C8        120.8(2)            .       .       .       yes
 C7      N1      C8        109.3(3)            .       .       .       yes
 C7      N2      C9        108.5(3)            .       .       .       yes
 C7      N2      C13       130.8(3)            .       .       .       yes
 C9      N2      C13       120.6(3)            .       .       .       yes
 V1      N3      C14       119.5(2)            .       .       .       yes
 V1      N3      C18       121.0(3)            .       .       .       yes
 C14     N3      C18       119.6(3)            .       .       .       yes
 O1      C1      C2        117.4(4)            .       .       .       yes
 O1      C1      C6        123.7(3)            .       .       .       yes
 C2      C1      C6        118.8(4)            .       .       .       no
 C1      C2      C3        120.6(4)            .       .       .       no
 C2      C3      C4        120.8(4)            .       .       .       no
 C3      C4      C5        119.7(4)            .       .       .       no
 C4      C5      C6        121.2(4)            .       .       .       no
```

```
 C1      C6      C5         118.6(3)              .       .       .          no
 C1      C6      C7         117.3(3)              .       .       .          no
 C5      C6      C7         123.8(4)              .       .       .          no
 N1      C7      N2         108.0(3)              .       .       .          yes
 N1      C7      C6         122.6(3)              .       .       .          yes
 N2      C7      C6         129.3(3)              .       .       .          yes
 N1      C8      C9         109.5(3)              .       .       .          yes
 N1      C8      C14        114.4(3)              .       .       .          yes
 C9      C8      C14        136.1(4)              .       .       .          no
 N2      C9      C8         104.6(3)              .       .       .          yes
 N2      C9      C10        118.4(3)              .       .       .          yes
 C8      C9      C10        136.9(3)              .       .       .          no
 C9      C10     C11        119.8(3)              .       .       .          no
 C10     C11     C12        119.9(3)              .       .       .          no
 C11     C12     C13        121.0(3)              .       .       .          no
 N2      C13     C12        119.9(3)              .       .       .          yes
 N3      C14     C8         112.4(3)              .       .       .          yes
 N3      C14     C15        121.5(3)              .       .       .          yes
 C8      C14     C15        126.1(3)              .       .       .          no
 C14     C15     C16        117.4(3)              .       .       .          no
 C15     C16     C17        121.1(4)              .       .       .          no
 C16     C17     C18        118.3(4)              .       .       .          no
 N3      C18     C17        122.1(4)              .       .       .          yes
 C1      C2      H2           119.71              .       .       .          no
 C3      C2      H2           119.69              .       .       .          no
 C2      C3      H3           119.53              .       .       .          no
 C4      C3      H3           119.63              .       .       .          no
 C3      C4      H4           120.11              .       .       .          no
 C5      C4      H4           120.17              .       .       .          no
 C4      C5      H5           119.44              .       .       .          no
 C6      C5      H5           119.34              .       .       .          no
 C9      C10     H10          120.07              .       .       .          no
 C11     C10     H10          120.16              .       .       .          no
 C10     C11     H11          120.03              .       .       .          no
 C12     C11     H11          120.04              .       .       .          no
 C11     C12     H12          119.47              .       .       .          no
 C13     C12     H12          119.50              .       .       .          no
 N2      C13     H13          119.98              .       .       .          no
 C12     C13     H13          120.15              .       .       .          no
 C14     C15     H15          121.35              .       .       .          no
 C16     C15     H15          121.27              .       .       .          no
 C15     C16     H16          119.42              .       .       .          no
 C17     C16     H16          119.49              .       .       .          no
 C16     C17     H17          120.84              .       .       .          no
 C18     C17     H17          120.82              .       .       .          no
 N3      C18     H18          118.91              .       .       .          no
 C17     C18     H18          118.95              .       .       .          no

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 N1      V1      O1      C1         -42.5(3)     .       .       .       .   no
 N3      V1      O1      C1         -78.4(5)     .       .       .       .   no
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 O1      V1      N1      C8        -159.2(3)     .       .       .       .   no
 O2      V1      N1      C7         -86.6(4)     .       .       .       .   no
 O2      V1      N1      C8          96.1(3)     .       .       .       .   no
 O3      V1      N1      C7         113.1(4)     .       .       .       .   no
 O3      V1      N1      C8         -64.3(4)     .       .       .       .   no
 N3      V1      N1      C7         179.4(4)     .       .       .       .   no
 N3      V1      N1      C8           2.0(3)     .       .       .       .   no
 O1      V1      N3      C14         37.8(5)     .       .       .       .   no
```

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 O1      V1      N3      C18       -143.1(4)     .       .       .       .   no
 O2      V1      N3      C14       -107.8(4)     .       .       .       .   no
 O2      V1      N3      C18         71.3(4)     .       .       .       .   no
 O3      V1      N3      C14        143.3(4)     .       .       .       .   no
 O3      V1      N3      C18        -37.7(4)     .       .       .       .   no
 N1      V1      N3      C14          0.5(3)     .       .       .       .   no
 N1      V1      N3      C18        179.5(4)     .       .       .       .   no
 V1      O1      C1      C2        -139.2(4)     .       .       .       .   no
 V1      O1      C1      C6          43.4(6)     .       .       .       .   no
 V1      N1      C7      N2        -176.7(3)     .       .       .       .   no
 V1      N1      C7      C6           6.2(7)     .       .       .       .   no
 C8      N1      C7      N2           0.9(5)     .       .       .       .   no
 C8      N1      C7      C6        -176.2(4)     .       .       .       .   no
 V1      N1      C8      C9         177.8(3)     .       .       .       .   no
 V1      N1      C8      C14         -4.0(5)     .       .       .       .   no
 C7      N1      C8      C9           0.0(5)     .       .       .       .   no
 C7      N1      C8      C14        178.2(4)     .       .       .       .   no
 C9      N2      C7      N1          -1.4(5)     .       .       .       .   no
 C9      N2      C7      C6         175.4(5)     .       .       .       .   no
 C13     N2      C7      N1         175.0(4)     .       .       .       .   no
 C13     N2      C7      C6          -8.2(8)     .       .       .       .   no
 C7      N2      C9      C8           1.3(5)     .       .       .       .   no
 C7      N2      C9      C10       -178.2(4)     .       .       .       .   no
 C13     N2      C9      C8        -175.5(4)     .       .       .       .   no
 C13     N2      C9      C10          5.0(6)     .       .       .       .   no
 C7      N2      C13     C12        178.0(5)     .       .       .       .   no
 C9      N2      C13     C12         -5.9(7)     .       .       .       .   no
 V1      N3      C14     C8          -2.5(5)     .       .       .       .   no
 V1      N3      C14     C15        177.6(3)     .       .       .       .   no
 C18     N3      C14     C8         178.4(4)     .       .       .       .   no
 C18     N3      C14     C15         -1.5(7)     .       .       .       .   no
 V1      N3      C18     C17       -178.1(4)     .       .       .       .   no
 C14     N3      C18     C17          1.0(7)     .       .       .       .   no
 O1      C1      C2      C3         178.6(5)     .       .       .       .   no
 C6      C1      C2      C3          -3.8(7)     .       .       .       .   no
 C2      C1      C6      C7         179.9(3)     .       .       .       .   no
 C2      C1      C6      C5           5.1(7)     .       .       .       .   no
 O1      C1      C6      C5        -177.5(4)     .       .       .       .   no
 O1      C1      C6      C7          -2.7(7)     .       .       .       .   no
 C1      C2      C3      C4           0.5(8)     .       .       .       .   no
 C2      C3      C4      C5           1.5(7)     .       .       .       .   no
 C3      C4      C5      C6          -0.2(7)     .       .       .       .   no
 C4      C5      C6      C1          -3.1(7)     .       .       .       .   no
 C4      C5      C6      C7        -177.6(4)     .       .       .       .   no
 C1      C6      C7      N1         -19.4(7)     .       .       .       .   no
 C1      C6      C7      N2         164.3(4)     .       .       .       .   no
 C5      C6      C7      N1         155.1(4)     .       .       .       .   no
 C5      C6      C7      N2         -21.2(8)     .       .       .       .   no
 N1      C8      C9      C10        178.6(5)     .       .       .       .   no
 C14     C8      C9      N2        -178.5(5)     .       .       .       .   no
 N1      C8      C9      N2          -0.8(5)     .       .       .       .   no
 C9      C8      C14     C15          1.4(9)     .       .       .       .   no
 C14     C8      C9      C10         0.9(10)     .       .       .       .   no
 N1      C8      C14     N3           4.0(6)     .       .       .       .   no
 N1      C8      C14     C15       -176.2(4)     .       .       .       .   no
 C9      C8      C14     N3        -178.4(5)     .       .       .       .   no
 C8      C9      C10     C11       -179.5(5)     .       .       .       .   no
 N2      C9      C10     C11         -0.2(7)     .       .       .       .   no
 C9      C10     C11     C12         -3.6(7)     .       .       .       .   no
 C10     C11     C12     C13          2.8(8)     .       .       .       .   no
 C11     C12     C13     N2           2.1(8)     .       .       .       .   no
 N3      C14     C15     C16          1.1(7)     .       .       .       .   no
 C8      C14     C15     C16       -178.7(5)     .       .       .       .   no
 C14     C15     C16     C17         -0.4(8)     .       .       .       .   no
 C15     C16     C17     C18         -0.1(8)     .       .       .       .   no
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loop_
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 V1      C15        3.495(5)                    .     3_666                no
 V1      C16        3.914(5)                    .     3_666                no
 V1      C14        3.785(4)                    .     3_666                no
 V1      H12          3.2427                    .     2_655                no
 V1      H13          2.9778                    .     2_655                no
 V1      H15          3.5010                    .     3_666                no
 O1      C15        3.357(6)                    .     3_666                no
 O1      C16        3.204(6)                    .     3_666                no
 O2      C10        3.061(6)                    .     3_766                no
 O2      C13        3.246(5)                    .     2_655                no
 O2      C3         3.310(5)                    .     3_665                no
 O2      C4         3.399(5)                    .     3_665                no
 O3      C15        3.072(5)                    .     3_666                no
 O3      C10        3.021(6)                    .     3_666                no
 O3      C14        3.409(5)                    .     3_666                no
 O3      C9         3.300(5)                    .     3_666                no
 O3      C13        2.994(5)                    .     2_655                no
 O3      C12        3.285(5)                    .     2_655                no
 O1      H12          2.7052                    .     2_655                no
 O2      H3           2.6650                    .     3_665                no
 O2      H10          2.4130                    .     3_766                no
 O2      H4           2.8483                    .     3_665                no
 O2      H13          2.6856                    .     2_655                no
 O3      H13          2.2299                    .     2_655                no
 O3      H12          2.8327                    .     2_655                no
 O3      H18          2.6116                    .       .                  no
 O3      H10          2.6333                    .     3_666                no
 O3      H15          2.7077                    .     3_666                no
 N1      C15        3.329(7)                    .     3_766                no
 N2      C16        3.316(6)                    .     3_766                no
 N3      C10        3.447(6)                    .     3_766                no
 N3      C8         3.409(6)                    .     3_666                no
 N2      H5           2.8878                    .       .                  no
 C1      C3         3.574(7)                    .     3_665                no
 C2      C3         3.545(7)                    .     3_665                no
 C3      C2         3.545(7)                    .     3_665                no
 C3      O2         3.310(5)                    .     3_665                no
 C3      C1         3.574(7)                    .     3_665                no
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 C5      C13        3.230(5)                    .       .                  no
 C7      C15        3.452(7)                    .     3_766                no
 C7      C16        3.352(7)                    .     3_766                no
 C7      C17        3.444(7)                    .     3_666                no
 C8      N3         3.409(6)                    .     3_666                no
 C8      C15        3.403(7)                    .     3_766                no
 C8      C14        3.379(7)                    .     3_766                no
 C8      C18        3.436(7)                    .     3_666                no
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 C9      C14        3.490(6)                    .     3_766                no
 C9      O3         3.300(5)                    .     3_666                no
 C9      C15        3.587(6)                    .     3_766                no
 C10     O3         3.021(6)                    .     3_666                no
 C10     O2         3.061(6)                    .     3_766                no
 C10     C15        3.563(5)                    .       .                  no
 C10     C18        3.482(7)                    .     3_766                no
 C10     N3         3.447(6)                    .     3_766                no
 C11     C18        3.534(7)                    .     3_766                no
 C12     O3         3.285(5)                    .     2_645                no
 C12     V1         3.785(4)                    .     2_645                no
 C13     C5         3.230(5)                    .       .                  no
 C13     O2         3.246(5)                    .     2_645                no
 C13     C17        3.504(7)                    .     3_766                no
 C13     O3         2.994(5)                    .     2_645                no
 C13     V1         3.657(4)                    .     2_645                no
 C14     C8         3.379(7)                    .     3_766                no
 C14     V1         3.785(4)                    .     3_666                no
 C14     O3         3.409(5)                    .     3_666                no
 C14     C9         3.490(6)                    .     3_766                no
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C15	C7	3.452(7)	.	3_766	no
C15	O1	3.357(6)	.	3_666	no
C15	O3	3.072(5)	.	3_666	no
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C15	V1	3.495(5)	.	3_666	no
C15	C8	3.403(7)	.	3_766	no
C15	C10	3.563(5)	.	.	no
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C16	O1	3.204(6)	.	3_666	no
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C17	C13	3.504(7)	.	3_766	no
C18	C9	3.456(7)	.	3_666	no
C18	C8	3.436(7)	.	3_666	no
C18	C11	3.534(7)	.	3_766	no
C18	C10	3.482(7)	.	3_766	no
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C3	H12	3.0560	.	4_454	no
C4	H18	2.8105	.	2_645	no
C5	H18	3.0389	.	2_645	no
C5	H13	2.7025	.	.	no
C6	H13	3.0253	.	.	no
C9	H15	3.0942	.	.	no
C10	H15	3.0025	.	.	no
C12	H4	2.9860	.	4_555	no
C13	H5	2.6488	.	.	no
C15	H10	3.0890	.	.	no
H2	C2	2.9629	.	3_565	no
H2	H2	2.4891	.	3_565	no
H3	H15	2.5378	.	1_454	no
H3	O2	2.6650	.	3_665	no
H4	H18	2.4073	.	2_645	no
H4	O2	2.8483	.	3_665	no
H4	C12	2.9860	.	4_554	no
H5	N2	2.8878	.	.	no
H5	C13	2.6488	.	.	no
H5	H13	2.0529	.	.	no
H10	C15	3.0890	.	.	no
H10	H15	2.3529	.	.	no
H10	O2	2.4130	.	3_766	no
H10	O3	2.6333	.	3_666	no
H12	V1	3.2427	.	2_645	no
H12	O1	2.7052	.	2_645	no
H12	O3	2.8327	.	2_645	no
H12	C3	3.0560	.	4_655	no
H13	C5	2.7025	.	.	no
H13	C6	3.0253	.	.	no
H13	H5	2.0529	.	.	no
H13	V1	2.9778	.	2_645	no
H13	O2	2.6856	.	2_645	no
H13	O3	2.2299	.	2_645	no
H15	C9	3.0942	.	.	no
H15	C10	3.0025	.	.	no
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H15	V1	3.5010	.	3_666	no
H15	O3	2.7077	.	3_666	no
H18	O3	2.6116	.	.	no
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#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
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C13     H13     O3          0.9492     2.2299   2.994(5)     136.92   2_645 yes

# End of Crystallographic Information File
#=================================================================================
# Dr. A.L.Spek, Laboratory of Crystal and Structural Chemistry                    #
# Bijvoet Center for Biomolecular Research, Utrecht University.                   #
# (Kruytgebouw, room N801), Padualaan 8, 3584 CH Utrecht, The Netherlands.        #
# E-mail: a.l.spek@chem.uu.nl       http://www.cryst.chem.uu.nl/                  #
#                                   http://www.cryst.chem.uu.nl/platon/           #
#                                   anonymous ftp: xraysoft.chem.uu.nl            #
# FAX   : (31)-30-2533940           PHONE : (31)-30-2532538/2533/3902/3502        #
#=================================================================================
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